SCHRÖDINGER OPERATORS WITH A_{∞} POTENTIALS

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ABSTRACT. We study the heat kernel p(x,y,t) associated to the real Schrödinger operator $H = -\Delta + V$ on $L^2(\mathbb{R}^n)$, $n \geq 1$. Our main result is a pointwise upper bound on p when the potential $V \in A_{\infty}$. In the case that $V \in RH_{\infty}$, we also prove a lower bound. Additionally, we compute p explicitly when V is a quadratic polynomial.

1. MOTIVATION AND RELATED WORK

1.1. Real Schrödinger operators. Schrödinger operators $H = -\Delta + V$ enjoy considerable interest due to their physical importance. For example, thousands of papers have been devoted to the study of quantal anharmonic oscillators, which feature H with potential $V(x) = x^2 + \lambda x^{2m}$. In general, given any $V \geq 0$ in $L^1_{loc}(\mathbb{R}^n)$, we can define H as an operator on $L^2(\mathbb{R}^n)$ through its Dirichlet form (see [ABA07]). This leads to an associated H-heat equation

$$\begin{cases} \partial_t u + Hu = 0 & \text{in } \mathbb{R}^n \times (0, \infty) \\ \lim_{t \to 0^+} u(x, t) = f(x) & \text{on } \mathbb{R}^n \end{cases}$$

where the limit is in $L^2(\mathbb{R}^n)$. General solutions to this equation are weak solutions (defined below) given by integration against a kernel p(x, y, t) called the heat kernel of H. Namely,

$$u(x,t) = e^{-tH} f(x) = \int_{\mathbb{R}^n} p(x,y,t) f(y) \, dy,$$

Nonnegativity of V implies a trivial Gaussian bound $p(x,y,t) \leq (4\pi t)^{-n/2} e^{-\frac{|x-y|^2}{4t}}$ (see [Dav89]). Looking closer, there is a diverse literature on upper bounds for p, mirroring the variety of interesting potentials to work with. A common reference point is Davies' results for H with continuous potentials diverging to infinity as $|x| \to \infty$; he established the qualitatively sharp bounds

$$p(x, y, t) \le c(t)\phi(x)\phi(y)$$

where ϕ is the L^2 -normalized ground state of H, and c(t) has an explicit description as $t \to 0$ (again see [Dav89]). For classes of potentials that are not as well-behaved, one still hopes to prove extra-Gaussian decay in terms of V, even if sharp results are not attainable.

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1.2. Connection with several complex variables. Our original motivation was the Kohn Laplacian \Box_b on a class of CR manifolds in \mathbb{C}^2 . For a subharmonic function ϕ , the three-dimensional CR manifold M defined by

$$M = \{(z, w) \in \mathbb{C}^2 : \operatorname{Im} w = \phi(z)\}\$$

is pseudoconvex, the complex analysis version of convexity. Since M does not depend on $\operatorname{Re} w$, we can analyze the Kohn Laplacian \square_b and the \square_b -heat kernel via a partial Fourier transform in $\operatorname{Re} w$. This has been carried out by several mathematicians, e.g., [Chr91, Rai06a, Rai06b, Rai07, Rai12, BR13, Ber96]. If, in addition, $\phi(z) = \phi(\operatorname{Re} z)$ only depends on $\operatorname{Re} z$, then Nagel observed that a partial Fourier transform in $\operatorname{Im} z$ reduces \square_b and its associated operators even further [Nag86]. If τ and η are the transform variables of $\operatorname{Re} w$ and $\operatorname{Im} z$, respectively, then

$$\widehat{\Box_b} = -\Delta + \phi'' \tau + (\eta - \tau \phi')^2,$$

an operator of the form H with $V = \phi''\tau + (\eta - \tau\phi')^2$. Since ϕ is convex (a subharmonic function of one variable is convex), $V \geq 0$ when $\tau \geq 0$. Nagel's observation about the reduced form of $\bar{\partial}_b$ and its associated operators when $\phi(z) = \phi(\text{Re } z)$ has been repeatedly exploited [Has94, HNW10, RT15]. Once we have sufficient estimates on H, we will be able to recover information about \Box_b , in the same spirit as [Rai12, BR13].

1.3. Potentials in reverse Hölder classes and A_{∞} . In this note, we focus on V belonging to the Muckenhoupt class A_{∞} [Muc72]. Membership in A_{∞} is equivalent to membership in some reverse Hölder class RH_q for q > 1, where RH_q is defined as follows.

Definition 1.1. For $1 < q \le \infty$, nonnegative $V \in L^q_{loc}(\mathbb{R}^n)$ belongs to the reverse Hölder class RH_q if there exists C > 0 such that for all cubes Q of \mathbb{R}^n ,

$$\left(\frac{1}{|Q|} \int_{Q} V^{q} dx\right)^{1/q} \le \frac{C}{|Q|} \int_{Q} V dx$$

where for $q = \infty$ the left hand side is the ess sup over Q. In particular, $A_{\infty} = \bigcup_{q>1} RH_q$.

Such potentials need not have uniform behavior at infinity, e.g., $V(x_1, x_2, x_3) = (x_1x_2x_3)^2$; and may have integrable singularities, e.g., $V(x) = |x|^{-\alpha}$ with $\alpha < n$. See Stein [Ste93] for further details. In [Kur00] Kurata proved, for $n \ge 2$ and $V \in RH_q$ with $q \ge n/2$, that

(1)
$$p(x,y,t) \le \frac{c_0}{t^{n/2}} e^{-c_2 \frac{|x-y|^2}{t}} \exp\left\{-c_1 (1 + m_V(x)^2 t)^{1/(2(k_0+1))}\right\}$$

where $m_V(x)$ is a function measuring the effective growth of V near x. This estimate gives a non-sharp order of decay for computable examples such as $V = |x|^{\alpha}$ where $\alpha > 0$; hence its primary interest lies in the diversity of potentials to which it applies. The natural question is whether we can go further to remove the limitations on n and q.

2. An Upper Bound for p when $V \in A_{\infty}$

We provide just such an analogue of (1) for all $n \ge 1$ and q > 1. Specifically, let

$$\operatorname{av}_{Z_r(x)} V = \frac{1}{|Z_r(x)|} \int_{Z_r(x)} V \, dx$$

denote the average of V over the cube $Z_r(x)$ centered at x with side length r. Then we establish the following.

Theorem 2.1. If $V \in A_{\infty}$, the heat kernel of the Schrödinger operator $H = -\Delta + V$ on $L^2(\mathbb{R}^n)$ satisfies

(2)
$$p(x,y,t) \le \frac{c_0}{t^{n/2}} e^{-c_2 \frac{|x-y|^2}{t}} \exp\left\{-c_1 m_\beta (t \text{ av}_{Z_{\sqrt{t}}(x)} V)^{1/2}\right\}$$

where $c_i > 0$ for i = 0, 1, 2 and $m_{\beta}(x) = x$ for $x \leq 1$ and $m_{\beta}(x) = x^{\beta}$ for $x \geq 1$. In particular, if $V \in A_p$, then one may take $\beta = \frac{2}{2 + n(p-1)}$.

To orient ourselves with how close our result is to being sharp, we provide the explicit heat kernel for quadratic polynomial V on \mathbb{R} .

Theorem 2.2. If $V(x) = \sum_{i=0}^{2} a_i x^i$ with $a_2 > 0$, then the heat kernel p(x, y, t) of the Schrödinger operator $H = -\Delta + V$ on $L^2(\mathbb{R}^n)$ is given by the formula

$$p(x,y,t) = \left(\frac{\sqrt{a_2} \operatorname{csch} 2\sqrt{a_2}t}{2\pi}\right)^{1/2} e^{\left(\frac{a_1^2}{4a_2} - a_0\right)t}$$

$$\cdot \exp\left\{-\frac{a_1^2}{4(\sqrt{a_2})^3} (\operatorname{coth} 2\sqrt{a_2}t - \operatorname{csch} 2\sqrt{a_2}t)\right\}$$

$$\cdot \exp\left\{-\frac{\sqrt{a_2}}{2} \left((x-y)^2 \operatorname{csch} 2\sqrt{a_2}t + (x^2+y^2)(\operatorname{coth} 2\sqrt{a_2}t - \operatorname{csch} 2\sqrt{a_2}t)\right)\right\}$$

$$\cdot \exp\left\{-\frac{a_1}{2\sqrt{a_2}} \left((x+y)(\operatorname{coth} 2\sqrt{a_2}t - \operatorname{csch} 2\sqrt{a_2}t)\right)\right\}$$

for $x, y \in \mathbb{R}^n$ and t > 0.

First, recall the asymptotics

- $\operatorname{csch}(t) \sim t^{-1} \text{ as } t \to 0^+ \text{ and } \operatorname{csch}(t) \sim e^{-t} \text{ as } t \to +\infty$
- $(\coth(t) \operatorname{csch}(t)) \sim t \text{ as } t \to 0^+ \text{ and } (\coth(t) \operatorname{csch}(t)) \sim 1 \text{ as } t \to +\infty,$

So a sharp upper bound for the above formula is essentially

(3)
$$p(x,y,t) \lesssim \begin{cases} t^{-1/2} e^{-c_0 \frac{|x-y|^2}{t}} \exp\left\{-c_1 t(x^2 + y^2)\right\} & t \le 1\\ e^{-c_2 t} \exp\left\{-c_3 (x^2 + y^2)\right\} & t > 1 \end{cases}$$

To compare this to Theorem 2.1, we rewrite (2) to include a decay term in y,

$$p(x, y, t) = p(x, y, t)^{1/2} \cdot p(y, x, t)^{1/2}$$

(4)
$$\lesssim t^{-1/2} e^{-c_1 \frac{|x-y|^2}{t}} \exp\left\{-c_2 \left[m_\beta (t \operatorname{av}_{Z_{\sqrt{t}}(x)} V)^{1/2} + m_\beta (t \operatorname{av}_{Z_{\sqrt{t}}(y)} V)^{1/2} \right] \right\}.$$

Taking n = 1 and assuming quadratic V(x), we have

$$\operatorname{av}_{Z_{\sqrt{t}}(x)} V = \frac{1}{\sqrt{t}} \int_{x-\frac{1}{2}\sqrt{t}}^{x+\frac{1}{2}\sqrt{t}} V(z) \, dz = a_2 \left(x^2 + \frac{t}{12} \right) + a_1 x + a_0.$$

Thus we see that (4) is no sharper than a bound of

$$p(x, y, t) \lesssim t^{-1/2} e^{-c_1 \frac{|x-y|^2}{t}} \exp\left\{-c_2 \left[m_\beta(t^{1/2}|x|+t) + m_\beta(t^{1/2}|y|+t)\right]\right\}.$$

When all of the three terms $\{\sqrt{t}, |x|, |y|\}$ are small, the Gaussian factor will essentially determine the size of both the above, and of (3). But when t > 1 and say |x| is the dominant

term, our upper bound can be no sharper than $\exp\{-c|x|^{2\beta}\}$, while (3) will have decay of the order $\exp\{-cx^2\}$. Hence the presence of the sublinear function m_{β} prevents our estimates from being attained. However, if V(x) is a strictly positive polynomial, β may be taken arbitrarily close to 1 since positive polynomials belong to RH_{∞} .

Before moving to the proof of Theorem 2.1, we also take a moment to sketch its strategy, which uses ideas of Shen [She95]. Fix $y \in \mathbb{R}^n$, and look at $p = p(\cdot, y, t)$ in a cylinder $Q \subset \mathbb{R}^n \times (0, \infty)$. Since p is a weak solution to $(\partial_t + H)u = 0$ in this cylinder, Moser's work on local boundedness implies $\sup_Q p$ is dominated by its L^2 norm over a slightly larger cylinder. Now take an increasing sequence of cylinders beginning with Q. Given appropriate Fefferman-Phong and Caccioppoli type inequalities, we can alternate upper bounds for p in terms of its L^2 energy and L^2 norm over this sequence of cylinders. Each iteration introduces another factor of a V-dependent weight in the evolving upper bound. When we conclude the iteration by applying the Gaussian bound on p, our result is extra-Gaussian decay in terms of V.

So there are three main ingredients: local boundedness, a Fefferman-Phong inequality valid for $V \in A_{\infty}$, and a Caccioppoli inequality for weak solutions to $(\partial_t + H)u = 0$. We introduce these items in Subsections 2.1, 2.2, and 2.3, respectively; then combine them for the proof in Section 3.

2.1. Local boundedness. Denote cylinders in $\mathbb{R}^n \times (0, \infty)$ with the notation,

$$Q_r(x_0, t_0) = B(x_0, r) \times I_{t_0, r} = B(x_0, r) \times (t_0 - r^2, t_0)$$

And consider weak solutions of $(\partial_t + H)u = 0$ as below,

Definition 2.3. A real-valued function u(x,t) is a weak solution to $(\partial_t + H)u = 0$ in $Q_r(x_0,t_0)$ if $u \in L^{\infty}(L^2(B(x_0,r));I_{t_0,r}) \cap L^2(H^1(B(x_0,r));I_{t_0,r})$ satisfies

(5)
$$\int_{B(x_0,r)} u(x,t)\phi(x,t) dx - \int_{t_0-r^2}^t \int_{B(x_0,r)} u(x,s)\partial_s \phi(x,s) dx ds + \int_{t_0-r^2}^t \int_{B(x_0,r)} (\nabla u(x,s) \cdot \nabla \phi(x,s) + V(x)u(x,s)\phi(x,s)) dx ds = 0$$

for $t_0 - r^2 < t \le t_0$ and for every $\phi(x, s) \in \mathcal{C}$, where

$$\mathcal{C} = \{ \phi \in L^2(H^1(B(x_0, r)); I_{t_0, r}) \text{ and } \partial_s \phi \in L^2(L^2(B(x_0, r); I_{t_0, r}); \phi(x, r_0 - r^2)) = 0 \}$$

In this setting Moser established the following fundamental result, which applies to $p(\cdot, y, t)$ because it is a weak solution of $(\partial_t + H)u = 0$ on every such cylinder (see [Bal77]).

Theorem 2.4 (Moser). Let $u \ge 0$ be a weak solution of $(\partial_t + H)u = 0$ in $Q_{2r}(x_0, t_0)$. There exists C > 0, depending only on $n \ge 1$, such that

(6)
$$\sup_{Q_{r/2}(x_0,t_0)} |u(x,t)| \le \left(\frac{C}{r^{n+2}} \iint_{Q_{2r/3}(x_0,t_0)} |u|^2 dx dt\right)^{1/2}$$

Sketch of proof. We give a very precise reference because this fact is so basic for us. Suppose $Q_{2r}(x_0, t_0) = B_2(0) \times (0, 4)$. Note that because $V \ge 0$, u is a weak subsolution of $(\partial_t - \Delta)u = 0$ in $Q_2(0, 4)$. So subsolution estimates for the heat equation apply. In particular, a slight

modification in the geometry of Moser's Theorem 1 in [Mos64] (see especially pp. 124-125) establishes

$$\sup_{Q_{1/2}(0,4)} |u(x,t)| \le \left(C \iint_{Q_{2/3}(0,4)} |u|^2 \, dx \, dt \right)^{1/2}$$

Translation invariance of the heat equation then implies the lemma with r=1, and the result for arbitrary r>0 follows from invariance of the heat equation under the scaling $x \to rx$, $t \to r^2t$.

2.2. A Fefferman-Phong inequality. Next we consider how to trade an L^2 norm bound like (6) for an L^2 energy bound by introducing a V-dependent weight. What follows is the p=2 case of Auscher and Ben Ali's "improved Fefferman-Phong inequality" from [ABA07].

Theorem 2.5 (Auscher, Ben Ali). Suppose $V \in A_{\infty}$. Then there are constants C > 0 and $\beta \in (0,1)$, depending only on $n \geq 1$ and the A_{∞} constant of V, such that for any cube $Z = Z_r(x_0)$ and $u \in C^1(\mathbb{R}^n)$ one has

(7)
$$\int_{Z} |\nabla u|^{2} + V |u|^{2} dx \ge C \frac{m_{\beta}(r^{2} \text{ av}_{Z} V)}{r^{2}} \int_{Z} |u|^{2} dx$$

where $m_{\beta}(x) = x$ for $x \leq 1$ and $m_{\beta}(x) = x^{\beta}$ for $x \geq 1$. In particular, if $V \in A_p$, then one may take $\beta = \frac{2}{2+n(p-1)}$.

The name comes from Fefferman and Phong's "Main Lemma" in [Fef83] for polynomial potentials V on \mathbb{R}^n , which concludes $\int_Z |\nabla u|^2 + V|u|^2 dx \gtrsim R^{-2} \int_Z |u|^2 dx$ for reasonable functions u(x). As we will show, Auscher and Ben Ali's work provides just the generalization we need to sharpen Moser's bound (6) to include effects of V.

2.3. A Caccioppoli inequality. Broadly speaking, a Caccioppoli inequality bounds the local energy of a weak solution to an elliptic or parabolic equation by its L^2 norm over a slightly larger set. This is what we need for the third ingredient of our iteration. The version we need also appears as Lemma 3 in [Kur00]; we state it here and provide a proof in Section 3 for completeness.

Lemma 2.6. Fix $\sigma \in (0,1)$. If u is a weak solution to $(\partial_t + H)u = 0$ in $Q_{2r}(x_0,t_0)$, then there exists C > 0, depending only on $n \ge 1$, such that

$$\sup_{t_0 - (\sigma r)^2 \le t \le t_0} \int_{B(x_0, \sigma r)} |u(x, t)|^2 dx + \iint_{Q_{\sigma r}(x_0, t_0)} \left(|\nabla u|^2 + V |u|^2 \right) dx ds \\
\le \frac{C}{(1 - \sigma)^2 r^2} \iint_{Q_r(x_0, t_0)} |u|^2 dx dt$$

3. Proof of The Upper Bound

We hope that the reader has gained some intuition for how these three main ingredients might be combined, and provide the details next.

Proof of Theorem 2.1. Fix $y \in \mathbb{R}^n$, and focus on the cylinder $Q_r(x,t)$ with $r = \sqrt{t/8}$. Write $u(\cdot,s) = p(\cdot,y,s)$ so that u is a weak solution to $(\partial_s + H)u = 0$ in $Q_{2r}(x,t)$. We will define

an increasing sequence of cylinders that starts with $Q_{2/3r}(x,t)$. In particular, choose $k \in \mathbb{N}$ and define

$$\rho_j = \frac{2}{3} + \left(\frac{j-1}{k}\right)\frac{1}{3}$$
 for $j = 1, 2, \dots, k+1$.

These $\rho_1, \ldots, \rho_{k+1}$ are a sequence of k scaling factors increasing from $\rho_1 = 2/3$ to $\rho_{k+1} = 1$. For each $j = 2, \ldots, k+1$, also define nonnegative cutoff functions $\chi_j(z) \in C_0^{\infty}(B(x, \rho_j r))$ and $\eta_j(s) \in C^{\infty}(\mathbb{R})$, bounded by 1 and satisfying

•
$$\chi_j \equiv 1 \text{ on } B(x, \rho_{j-1}r), \ |\nabla \chi_j| \le \frac{Ck}{r}$$

•
$$\eta_j \equiv 0 \text{ for } t \le t_0 - (\rho_j r)^2, \ \eta_j \equiv 1 \text{ for } t \ge t_0 - (\rho_{j-1} r)^2, \ |\eta_j'| \le \frac{Ck}{r^2}.$$

Note in particular that supp $\chi_j \eta_j \subset B(x,r) \times [t_0 - r^2, \infty)$.

Consider one of these cylinders $Q_{\rho_{j+1}r}(x,t)$, where $j=1,\ldots,k$. Take the radius r in Lemma 2.6 to be our $\rho_{j+1}r$; and take the scaling factor σ in Lemma 2.6 to be $\frac{\rho_j}{\rho_{j+1}}$. Then applying the Caccioppoli inequality,

$$\iint_{Q_{\rho_{j+1}r}(x,t)} \left(|\nabla u|^2 \chi_{j+1}^2 \eta_{j+1}^2 + V u^2 \chi_{j+1}^2 \eta_{j+1}^2 \right) dz \, ds \le \frac{Ck^2}{r^2} \iint_{Q_{\rho_{j+1}r}(x,t)} |u|^2 \, dz \, ds.$$

And from Cauchy's inequality

$$|\nabla(\eta_{j+1}u\chi_{j+1})|^2 \le 2|\nabla u|^2\eta_{j+1}^2\chi_{j+1}^2 + 2|u|^2|\nabla\chi_{j+1}|^2\eta_{j+1}^2.$$

So using the bounds on $|\nabla \chi_{j+1}|$ and η_{j+1} , increasing C as necessary, we also have

(8)
$$\int_{t-(\rho_{j+1}r)^2}^t \int_{B_{\rho_{j+1}r}(x)} \left(|\nabla(\eta_{j+1}u\chi_{j+1})|^2 + V|u|^2 \chi_{j+1}^2 \eta_{j+1}^2 \right) dz ds$$
$$\leq \frac{Ck^2}{r^2} \iint_{Q_{\rho_{j+1}r}(x,t)} |u|^2 dz ds.$$

Now note that on the left-hand side of this inequality, we may apply the Fefferman-Phong inequality (7) to the integral in the space directions. We do this on a cube containing the support of χ_{j+1} , namely $Z_{2r}(x)$,

$$\int_{B_{\rho_{j+1}r}(x)} \left(|\nabla(\eta_{j+1}u\chi_{j+1})|^2 + V|u|^2 \chi_{j+1}^2 \eta_{j+1}^2 \right) dz$$

$$= \int_{Z_{2r}(x)} \left(|\nabla(\eta_{j+1}u\chi_{j+1})|^2 + V|u|^2 \chi_{j+1}^2 \eta_{j+1}^2 \right) dz$$

$$\geq \frac{C}{r^2} m_\beta(r^2 \operatorname{av}_{Z_{2r}(x)} V) \int_{B_{\rho_{j+1}r}(x)} |\eta_{j+1}u\chi_{j+1}|^2 dz.$$

Combined with (8), this implies

$$\int_{t-(\rho_{j+1}r)^2}^t \frac{m_{\beta}(r^2 \operatorname{av}_{Z_{2r}(x)} V)}{r^2} \int_{B_{\rho_{j+1}r}(x)} |\eta_{j+1} u \chi_{j+1}|^2 dz ds \leq \frac{Ck^2}{r^2} \iint_{Q_{\rho_{j+1}r}(x,t)} |u|^2 dz ds,$$

and hence

$$\iint_{Q_{\rho_{j+1}r}(x,t)} |\eta_{j+1}u\chi_{j+1}|^2 dz ds \le \frac{Ck^2}{m_{\beta}(r^2 \operatorname{av}_{Z_{2r}(x)} V)} \iint_{Q_{\rho_{j+1}r}(x,t)} |u|^2 dz ds.$$

In other words, combining Lemma 2.6 and Theorem 2.5 lets us directly relate the L^2 norm of u at the the ρ_j scaling to the ρ_{j+1} scaling,

$$\iint_{Q_{\rho_{j}r}(x,t)} |u|^2 dz ds \le \iint_{Q_{\rho_{j+1}r}(x,t)} |\eta_{j+1}u\chi_{j+1}|^2 dz ds$$

$$\le \frac{Ck^2}{m_{\beta}(r^2 \operatorname{av}_{Z_{2r}(x)} V)} \iint_{Q_{\rho_{j+1}r}(x,t)} |u|^2 dz ds.$$

Starting with j = 1 and iterating this relation k times yields

$$\iint_{Q_{2r/3}(x,t)} |u|^2 dz ds \le \frac{C^k k^{2k}}{m_\beta (r^2 \operatorname{av}_{Z_{2r}(x)} V)^k} \iint_{Q_r(x,t)} |u|^2 dz ds$$

Which substituted into Moser's estimate (6) yields

(9)
$$\sup_{(z,s)\in Q_{r/2}(x,t)} |u| \lesssim \frac{C^{k/2}k^k}{m_{\beta}(r^2 \operatorname{av}_{Z_{2r}(x)} V)^{k/2}} \left(\frac{1}{r^{n+2}} \iint_{Q_r(x,t)} |u|^2 dz ds\right)^{1/2}$$

with the suppressed constant independent of k. By [BR13, Proposition 3.1], it follows immediately that with c_1 in that proposition as $(eC)^{-1}$,

$$\sup_{(z,s)\in Q_{r/2}(x,t)} |u| \le c_0 \exp\left\{-c_1 m_\beta (r^2 \operatorname{av}_{Z_{2r}(x)} V)^{1/2}\right\} \left(\frac{1}{r^{n+2}} \iint_{Q_r(x,t)} |u|^2 dz ds\right)^{1/2},$$

and recalling that $r=\sqrt{t/8}$ and $u(\cdot,s)=p(\cdot,y,s)$

(10)
$$p(x, y, t) \le c_0 \exp\left\{-c_1 m_\beta (t \operatorname{av}_{Z_{\sqrt{t/2}}(x)} V)^{1/2}\right\} \left(\frac{1}{t^{(n+2)/2}} \iint_{Q_{\sqrt{t/8}}(x,t)} |p|^2 dz ds\right)^{1/2}.$$

Because A_{∞} potentials are doubling, in (10) we can now replace the average of V over $Z_{\sqrt{t/2}}(x)$ with its average over $Z_{\sqrt{t}}(x)$, scaling c_1 appropriately.

The final step is to incorporate the Gaussian bound on the heat kernel

(11)
$$p(x, y, t) \lesssim t^{-n/2} \exp(-|x - y|^2/4t).$$

In particular, if $|x-y| \approx \sqrt{t}$, we lose nothing by using $p \lesssim t^{-n/2}$ inside the integral in (10). Because $|Q_r| \approx r^{n+2}$, this gives

(12)
$$p(x, y, t) \le \frac{c_0}{t^{n/2}} \exp\left\{-c_1 m_\beta (t \text{ av}_{Z_{\sqrt{t}}(x)} V)^{1/2}\right\}.$$

On the other hand, if $\sqrt{t} \ll |x-y|$ then $p \lesssim t^{-n/2}$ is a very poor estimate. We would be better off just using (11) directly. So the upper bound of the theorem is a compromise that follows from writing

$$p(x, y, t) = p(x, y, t)^{1/2} \cdot p(x, y, t)^{1/2}$$

and then applying (11) to the first term in the product, (12) to the second. \Box

Proof of Lemma 2.6. First, the argument in §9 of [Aro67] allows us to assume that u has a strong derivative $\partial_t u \in L^2(Q_{2r}(x_0, t_0))$. Now choose nonnegative cutoff functions $\chi(x) \in C_0^{\infty}(B(x_0, r))$ and $\eta(s) \in C^{\infty}(\mathbb{R})$, bounded above by 1 and satisfying

•
$$\chi(x) \equiv 1 \text{ on } B(x_0, \sigma r), \ |\nabla \chi(x)| \le \frac{C}{(1-\sigma)r};$$

•
$$\eta(s) \equiv 0 \text{ for } s \le t_0 - r^2, \ \eta(s) \equiv 1 \text{ for } s \ge t_0 - (\sigma r)^2, \ |\eta'(s)| \le \frac{C}{(1 - \sigma)r^2}.$$

Fix $t \in [t_0 - (\sigma r)^2, t_0]$. Note that the test function $\eta^2(s)\chi^2(x)u(x, s)$ belongs to the class \mathcal{C} specified in Definition 2.3. Hence we may use this function for $\phi(x, s)$ in (5). This yields, since $\eta(t) = 1$,

(13)
$$\int_{B(x_0,r)} u^2 \chi^2 dx - \int_{t_0-r^2}^t \int_{B(x_0,r)} (u^2 (2\eta \eta') \chi^2 + (u \partial_s u) \eta^2 \chi^2) dx ds + \int_{t_0-r^2}^t \int_{B(x_0,r)} ((\nabla u \cdot \nabla \chi^2) \eta^2 u + |\nabla u|^2 \eta^2 \chi^2 + V u^2 \eta^2 \chi^2) dx ds = 0.$$

Note that the second integral in (13) may be written as

$$\int_{t_0-r^2}^t \int_{B(x_0,r)} \frac{1}{2} \partial_s(u^2 \eta^2 \chi^2) \, dx \, ds + \int_{t_0-r^2}^t \int_{B(x_0,r)} (u^2(\eta \, \eta') \chi^2 \, dx \, ds.$$

And by the bounded convergence theorem we may interchange integration and differentiation in the first term above, so because $\eta(t_0 - r^2) = 0$ it follows

$$\int_{t_0-r^2}^t \int_{B(x_0,r)} \frac{1}{2} \partial_s (u^2 \eta^2 \chi^2) \, dx \, ds = \frac{1}{2} \int_{B(x_0,r)} u^2 \chi^2 \, dx.$$

Substituting these observations into (13), we obtain

$$(14) \quad \frac{1}{2} \int_{B(x_0,r)} u^2 \chi^2 \, dx + \int_{t_0-r^2}^t \int_{B(x_0,r)} (|\nabla u|^2 \eta^2 \chi^2 + V u^2 \eta^2 \chi^2) \, dx \, ds$$

$$= \int_{t_0-r^2}^t \int_{B(x_0,r)} (u^2 \chi^2 \eta \, \eta' - (\nabla u \cdot \nabla \chi^2) \, \eta^2 u) \, dx \, ds$$

Since t was arbitrary and $V \geq 0$, we next conclude

$$\sup_{t_0 - (\sigma r)^2 \le t \le t_0} \frac{1}{2} \int_{B(x_0, r)} u^2 \chi^2 \, dx \le \iint_{Q_r(x_0, t_0)} \left(u^2 |\eta'| + |\nabla u| \chi \, \eta^2 \, |u| |\nabla \chi| \right) dx \, ds.$$

In the second term of the righthand integral we apply Cauchy's inequality $ab \leq \frac{a^2}{2} + \frac{b^2}{2}$, using $a = |\nabla u|\chi$, $b = |u||\nabla \chi|$. It follows

$$\sup_{t_0 - (\sigma r)^2 \le t \le t_0} \frac{1}{2} \int_{B(x_0, r)} u^2 \chi^2 \, dx \le \iint_{Q_r(x_0, t_0)} u^2 |\eta'| \, dx \, ds + \frac{1}{2} \iint_{Q_r(x_0, t_0)} \chi^2 \eta^2 |\nabla u|^2 \, dx \, ds + \frac{1}{2} \iint_{Q_r(x_0, t_0)} |u|^2 |\nabla \chi|^2 \eta^2 \, dx \, ds$$

And from the bounds on $|\nabla \chi|$, η , and $|\eta'|$,

(15)
$$\sup_{t_0 - (\sigma r)^2 \le t \le t_0} \int_{B(x_0, r)} u^2 \chi^2 dx$$

$$\le \frac{C}{(1 - \sigma)^2 r^2} \iint_{Q_r(x_0, t_0)} u^2 dx ds + \iint_{Q_r(x_0, t_0)} \chi^2 \eta^2 |\nabla u|^2 dx ds$$

To complete the proof we make another application of (14), this time with $t = t_0$. The positivity of the leftmost integral and the bounds on χ , η , and $|\eta'|$ yield

$$\iint_{Q_r(x_0,t_0)} \left(|\nabla u|^2 \chi^2 \, \eta^2 + V u^2 \chi^2 \eta^2 \right) dx \, ds
\leq \frac{C}{(1-\sigma)r^2} \iint_{Q_r(x_0,t_0)} u^2 \, dx \, ds + \iint_{Q_r(x_0,t_0)} |\nabla u| \chi \, \eta^2 \, |u| |\nabla \chi| \, dx \, ds$$

And the above use of Cauchy's inequality gives, after rearranging, absorbing terms, and possibly increasing C,

(16)
$$\iint_{Q_r(x_0,t_0)} \chi^2 \eta^2 |\nabla u|^2 dx ds + \iint_{Q_r(x_0,t_0)} V u^2 \chi^2 \eta^2 dx ds$$

$$\leq \frac{C}{(1-\sigma)^2 r^2} \iint_{Q_r(x_0,t_0)} u^2 dx ds$$

Combining (15) and (16) and restricting the lefthand integrals to where the cutoff functions are unity yields the lemma. Note that (16) is all that is needed for the proof of Theorem (2.1).

Proof of Theorem 2.2. It suffices to treat the case $a_0 = 0$, because

$$[\partial_t - \Delta + (a_2 x^2 + a_1 x + a_0)] u = e^{-a_0 t} [\partial_t - \Delta + (a_2 x^2 + a_1 x)] e^{a_0 t} u.$$

So if $p_0(x, y, t)$ is the heat kernel for the operator with potential $V(x) = \sum_{i=1}^2 a_i x^i$, then $e^{-a_0 t} p_0(x, y, t)$ is directly checked to be the heat kernel when $V(x) = \sum_{i=0}^2 a_i x^i$.

Several approaches to the calculation are possible. Interpreting p(x, y, t) as the transition probability of a system from state x to state y in time t, the kernel is determined by a certain path integral of the Lagrangian given by $(-\Delta + V)$. For quadratic V this path integral can then be computed using the van Vleck determinant (see [Vis93] for details.) Another possibility is to begin with the Mehler kernel of the harmonic oscillator (see again [Dav89]) and study the behavior of this kernel under appropriate scalings and translations of the harmonic oscillator. Our method, requiring rather less theory than either of the above, is to take from [Bea99] the ansatz

$$p(x,y,t) = \phi(t) \exp\left\{-\frac{1}{2}\left(\alpha(t)x^2 + \gamma(t)y^2 + 2\beta(t)xy\right)\right\} \exp\left\{-\mu(t)x - \nu(t)y\right\}.$$

We then simply attempt to enforce on this ansatz the two conditions

(18)
$$\begin{cases} (\partial_t + H)p(\cdot, y, t) = 0 & \text{on } \mathbb{R} \times (0, \infty) \\ \lim_{t \to 0^+} p(x, y, t) = \delta(x - y) & \text{in } L^1(\mathbb{R}) \end{cases}$$

The differential condition in (18) yields a system of six ODE's in t.

$$\alpha' = -2\alpha^2 + 2a_2$$

$$\beta' = -2\alpha\beta$$

$$(21) \gamma' = -2\beta^2$$

$$(23) \nu' = -2\mu\beta$$

$$\phi'/\phi = -\alpha + \mu^2.$$

These equations are solvable, in order, by elementary methods. The constants of integration must be chosen according to the second condition in (18). For $\beta(t)$ this is actually easy to do, but in solving the remaining equations we set constants of integration to zero and identify their true values only after the functional form of p(x, y, t) is known. Also, the singularity condition of (18) is equivalent to two properties. First,

$$\lim_{t \to 0^+} p(x, y, t) = 0$$

whenever $x \neq y$; and, second,

$$\lim_{t \to 0^+} \int_{\mathbb{R}} p(x, y, t) \, dy = 1$$

for any $x \in \mathbb{R}$.

The result follows from elementary, though tedious, computations.

4. A Lower Bound for p when $V \in RH_{\infty}$

For V which belongs to a local Kato class and decays or is L^{∞} bounded at infinity, Zhang and Zhao [ZZ00] proved the attractive lower bound

$$p(x,y,t) \ge \begin{cases} \frac{c_1}{t^{n/2}} e^{-c_2 K_{V^+}(t)} & |x-y|^2 \le t \\ \frac{c_1}{t^{n/2}} e^{-c_2 \frac{|x-y|^2}{t}} [1 + K_{V^+}(\frac{t^2}{|x-y|^2})] & |x-y|^2 \ge t \end{cases}$$

where

$$K_V(t) = \sup_{x} \int_0^t \int_{\mathbb{R}^n} \frac{1}{(t-s)^{n/2}} e^{-c\frac{|x-y|^2}{t-s}} |V(y)| \, dy \, ds.$$

But to our knowledge, the case with V unbounded near infinity has not received any attention in the literature. So here we provide a lower bound for p whose dependence on V is analogous to the V-dependent decay of Theorem 2.1. However, it applies only for $V \in RH_{\infty}$, the most tractable reverse Hölder class.

Theorem 4.1. If $V \in RH_{\infty}$, the heat kernel of the Schrödinger operator $H = -\Delta + V$ on $L^2(\mathbb{R}^n)$ satisfies with $0 < \kappa < 1$ fixed

(25)
$$p(x,y,t) \ge \begin{cases} \frac{c_0}{t^{n/2}} \exp\{-c_1 t \operatorname{av}_{Z_{\sqrt{t}}(x)} V\} & |x-y| < \kappa \sqrt{t} \\ \frac{c_0}{t^{n/2}} e^{-c_3 \frac{|x-y|^2}{t}} \exp\{-c_1 t (c_2^{\frac{|x-y|^2}{t}} \operatorname{av}_{Z_{t/|x-y|}(x)} V)\} & |x-y| \ge \kappa \sqrt{t} \end{cases}$$

for some constants $c_i > 0$ for i = 0, 1, 2, 3.

The idea of the proof is to establish a bridge between p and the heat kernel of an appropriate Dirichlet Laplacian, where van den Berg's results in [vdB90] can be applied. We will do this in Section 5 using the semigroup property of p(x, y, t), a parabolic maximum principle, and a lemma that relates the averages of a doubling measure over nested cubes. Let us first review our technical devices and van den Berg's estimates.

4.1. The semigroup property.

Lemma 4.2. Let p(x, y, t) be the heat kernel of a Schrödinger operator H on $L^2(\mathbb{R}^n)$ with locally integrable nonnegative potential. Then

$$p(x, y, t + s) = \int_{\mathbb{R}^n} p(x, z, t) p(z, y, s) dz$$

for all $x, y \in \mathbb{R}^n$ and s, t > 0.

This restates the standard fact that e^{-Ht} is a semigroup, but in the precise form we will need it. For an off-diagonal estimate of p(x, y, t), we will invoke Lemma 4.2 repeatedly to write p(x, y, t) as an iterated integral of many "copies" of itself at earlier times. Our on-diagonal bounds will then apply to these copies when they are restricted to appropriately small regions in space.

4.2. A maximum principle. The following maximum principle will connect the heat kernel of $H = -\Delta + V$ to that of an appropriate Dirichlet Laplacian. Note that we need the local boundedness of V implied by membership in RH_{∞} .

Theorem 4.3. Suppose $V \geq 0$ is bounded in a cylinder $Q = Q_r(x_0, t_0)$ and $u \in C(\overline{Q})$ is a weak solution of $(\partial_t + H)u = 0$ in Q. Then

$$\sup_{Q} u \le \sup_{\partial Q} u_{+} \quad and \quad \inf_{Q} u \ge \inf_{\partial Q} u_{-}.$$

If u is only a weak supersolution of the same equation in Q, then we still have the second conclusion.

Since we cannot assume u is a classical solution in Q, the proof is rather involved and best accomplished through functional analytic machinery. Details may be found in [KJN06].

4.3. A lemma for doubling measures. The following useful lemma comes from Christ [Chr91], and allows us to compare the averages of V over two cubes whose centers are some distance from each other.

Lemma 4.4. For any doubling measure ω on \mathbb{R}^n , there exist positive $C < \infty$ and $\epsilon < 1$ such that for any cubes $Z' \subset Z$

$$\int_{Z'} d\omega \le C \left(\frac{|Z'|}{|Z|}\right)^{\epsilon} \int_{Z} d\omega$$

where e.g., |Z| denotes the Euclidean measure of Z.

4.4. Estimates on the Dirichlet heat kernel. Now we come to van den Berg's results on Dirichlet heat kernels. Their statement differs somewhat for the n = 1 and $n \ge 2$ cases. In the latter case we need the following definition.

Definition 4.5. Fix an open set $D \subset \mathbb{R}^n$, where $n \geq 2$. Given $\epsilon > 0$, let D_{ϵ} be the points in D at least distance ϵ from the boundary; and let $d_{\epsilon}(x,y)$ for $x,y \in D$ be the infimum of lengths of arcs in D_{ϵ} with endpoints x and y. When $d_{\epsilon}(x,y) < \infty$, let γ_{ϵ} be a minimal geodesic from x to y and define

$$\alpha(\gamma_{\epsilon}) = \int_{s: \gamma_{\epsilon}(s) \in D_{\epsilon}} \left| \frac{d^{2} \gamma_{\epsilon}(s)}{ds^{2}} \right| ds.$$

Theorem 4.6 (van den Berg). Suppose D is an open set in \mathbb{R}^n with $n \geq 2$. Given $\epsilon > 0$, $0 < \delta \leq \epsilon$, $x \in D$, $y \in D$ such $d_{\epsilon}(x, y) < \infty$, it holds for all t > 0

$$\Gamma_D(x,y,t) \ge \frac{C}{t^{n/2}} e^{-\frac{\pi^2 n^2 t}{4\epsilon^2}} \exp\left\{-\frac{d_{\epsilon}(x,y)^2 (1 + 2\delta\alpha(\gamma_{\epsilon}) d_{\epsilon}(x,y))}{4t}\right\}$$

where Γ_D is the heat kernel of $-\Delta$ on D with Dirichlet boundary conditions and C < 1 is a positive constant depending only on n.

When using Theorem 4.6 we will always choose D to be a ball, so that D_{ϵ} is also a ball and

$$\gamma_{\epsilon}(s) = x + \frac{s}{|y - x|}(y - x).$$

Hence $\alpha(\gamma_{\epsilon})$ will always vanish in our applications.

When n = 1, van den Berg obtained a lower bound on Γ_D from ingenious use of a special function identity and the eigenfunction expansion of the Dirichlet heat kernel on an interval. Namely,

Proposition 4.7 (van den Berg). Suppose $D \subset \mathbb{R}$ is an interval, and for some x < y and $\epsilon > 0$ we have $(x - \epsilon, y + \epsilon) \subset D$. Then for all t > 0

$$\Gamma_D(x, y, t) \ge \frac{C}{t^{1/2}} e^{-\frac{|x-y|^2}{4t}} (1 - 2e^{-\frac{\epsilon^2}{t}})$$

where Γ_D is the heat kernel of $-\Delta$ on D with Dirichlet boundary conditions and C < 1 is a positive constant depending only on n.

5. Proof of the Lower Bound

Proof of Theorem 4.1. First suppose $|x-y| < \frac{1}{8}\sqrt{t}$. We consider the ball $B = B_{\sqrt{t}}(x)$. Let H_B be the restriction of the operator H to B with Dirichlet boundary conditions; and let $p_B(x,y,t)$ be the associated heat kernel. Note that $u(\cdot,t) = p(\cdot,y,t) - p_B(\cdot,y,t)$ is a weak solution to $(\partial_t + H)u = 0$ on $B \times (0,\infty)$, for any $y \in B$. And because $p_B(\cdot,y,t)$ vanishes on ∂B , u is nonnegative on the boundary, implying by the maximum principle that

(26)
$$p(x, y, t) \ge p_B(x, y, t) \quad \text{in } B \times B \times (0, \infty)$$

since the choice of $y \in B$ was arbitrary.

Now we use again the hypothesis that $V \in RH_{\infty}$. With C > 0 the RH_{∞} constant of V, we have for $M = C \operatorname{av}_{Z_{2,\sqrt{I}}(x)} V$ that $V \leq M$ in B. Let H_D^M be the operator $(-\Delta + M)$ restricted

to B with Dirichlet boundary conditions; so its heat kernel is just $e^{-Mt}\Gamma_D$, where Γ_D is the heat kernel of the Dirichlet Laplacian on B. Now for $y \in B$ set

$$w(x,t) = p_B(x,y,t) - e^{-Mt} \Gamma_D(x,y,t).$$

Then $w \equiv 0$ on $\partial B \times (0, \infty)$, and inside B we have for any t > 0

$$(\partial_t + H_D^M)w = (\partial_t - \Delta + M)p_B = (M - V)p_B \ge 0.$$

So w is a supersolution of $(\partial_t + H_B^M)$ in the cylinder $Q = B \times (0, \infty)$, vanishing on the boundary, and by the maximum principle satisfies

$$p_B(x, y, t) \ge e^{-Mt} \Gamma_D(x, y, t)$$
 in $B \times B \times (0, \infty)$

since $y \in B$ was arbitrary.

Applying either Proposition 4.7 or Theorem 4.6 with $\epsilon = \frac{7}{8}\sqrt{t}$, we obtain from the preceding inequality and (26) that

(27)
$$p(x, y, t) \ge \frac{c_0}{t^{n/2}} \exp\left\{-c_1 t \operatorname{av}_{Z_{2\sqrt{t}}(x)} V\right\}$$

where $c_0 < 1$ is a positive constant depending only on n, and c_1 is just the RH_{∞} constant of V. Because V is doubling, we may also increase c_1 and replace the cube $Z_{2\sqrt{t}}(x)$ with $Z_{\sqrt{t}}(x)$. These on-diagonal bounds conclude the first part of the proof.

Off-diagonal bounds come next. Assume $|x-y| \ge \frac{1}{8}\sqrt{t}$. We begin by considering the line segment from x to y given by

$$l(s) = x + s \frac{y - x}{|y - x|}, \quad s \in [0, |y - x|].$$

We will partition this segment by a sequence of M+1 points $\{x_i\}_{i=0}^M$; the sequence is determined by the requirement that $|x_i - x_{i+1}| = \frac{|y-x|}{M}$, where M is the smallest integer satisfying

$$\frac{|y-x|}{M} < \frac{1}{16}\sqrt{\frac{t}{M}} \Leftrightarrow \frac{256|y-x|^2}{t} < M$$

Now directly from Lemma 4.2 we have

$$p(x, y, t) = \int_{\mathbb{R}^n} p(x, z_1, t/M) p(z_1, y, (M-1)t/M) dz_1$$

and applying the semigroup property in the same way to the right-most integrand, (M-1) times, we get an iterated integral

$$p(x,y,t) = \int_{\mathbb{R}^n} \cdots \int_{\mathbb{R}^n} p(x,z_1,t/M) \cdots p(z_{M-1},y,t/M) dz_1 \cdots dz_{M-1}$$

Upon restricting each dz_i integral to $Z_i = Z_{\sigma\sqrt{t/M}}(x_i)$ with $0 < \sigma < 1$ such that

$$z_i \in Z_i \text{ and } z_{i+1} \in Z_{i+1} \Rightarrow |z_i - z_{i+1}| < \frac{1}{8} \sqrt{t/M}$$

we then obtain

(29)
$$p(x,y,t) \ge \int_{Z_1} \cdots \int_{Z_{M-1}} p(x,z_1,t/M) \cdots p(z_{M-1},y,t/M) dz_1 \cdots dz_{M-1}$$

And now our on-diagonal lower bounds apply to each term in the integrand.

That is, we have for each i = 0, ..., M-1 that

$$p(z_i, z_{i+1}, t/M) \ge c_0 \left(\frac{M}{t}\right)^{n/2} \exp\left\{-c_1 \frac{t}{M} \operatorname{av}_{Z_{\sigma\sqrt{t/M}}(z_i)} V\right\}.$$

To assimilate these into a single lower bound for p(x, y, t), we use Lemma 4.4. In particular we see that

$$\int_{Z_{\sigma\sqrt{t/M}}(z_i)} V \le C \left(\frac{1}{2^n}\right)^{\epsilon} \int_{Z_{2\sigma\sqrt{t/M}}(x_i)} V$$

$$\le C \int_{Z_i} V$$

and iterating this inequality up to M times (if i = M - 1) we may even conclude

$$\int_{Z_{\sigma\sqrt{t/M}}(z_i)} V \le C^M \int_{Z_0} V = C^M \int_{Z_{\sigma\sqrt{t/M}}(x)} V.$$

So in fact we have a lower bound, uniform in i, of

$$p(z_i, z_{i+1}, t/M) \ge c_0 \left(\frac{M}{t}\right)^{n/2} \exp\left\{-c_1 \frac{t}{M} C^M \operatorname{av}_{Z_{\sigma\sqrt{t/M}}(x)} V\right\}$$

It now just remains to apply this to each term in the integrand of (29). This yields

$$p(x, y, t) \ge \prod_{i=0}^{M-1} c_0 \left(\frac{M}{t}\right)^{n/2} \exp\left\{-c_1 \frac{t}{M} C^M \operatorname{av}_{Z_{\sigma\sqrt{t/M}}(x)} V\right\} \cdot \prod_{i=1}^{M-1} |Z_{\sigma\sqrt{t/M}}(x_i)|$$

$$\ge \frac{\sigma^{-1}}{t^{n/2}} M^{n/2} (\sigma c_0)^M \exp\left\{-c_1 t \left(C^M \operatorname{av}_{Z_{\sigma\sqrt{t/M}}(x)} V\right)\right\}.$$

Because $c_0 < 1$ and $\sigma < 1$, the factor $M^{n/2}(\sigma c_0)^M$ gives exponential decay in M; and by (28), M is comparable to $\frac{|x-y|^2}{t}$. Increasing constants as necessary and using Christ's lemma to replace M with $\frac{|x-y|^2}{t}$ yields (25) with $\kappa = 1/8$.

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